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Synthesis and structure of cyclopropenone π-complexes with pentacarbonyliron(0) and hexacarbonyltungsten(0). Hydrophosphorylation of cyclopropenone in the transition metal coordination sphere

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Abstract

New π-complexes of pentacarbonyliron(0) and hexacarbonyltungsten(0) containing η 2-coordinated cyclopropenone molecules were synthesized. The geometric, electronic structure, and energy parameters of the coordinated cyclic oxo diene were determined by nonempirical quantum-chemical methods. According to the theoretical and experimental (IR and NMR) data, the conjugation between the double carbon-carbon and carbon-oxygen bonds is broken as a result of coordination. The coordinated cyclopropenone reacts with dialkyl hydrogen phosphites to give the corresponding α-hydroxyphosphonate via addition at the carbonyl group, whereas hydrophosphorylation of the free ligand occurs at the double carbon-carbon bond.

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